Artificial intelligence and machine learning■aided drug discovery in central nervous system diseases: State■of■the■arts and future directions

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Abstract

Neurological disorders significantly outnumber diseases in other therapeutic areas. However, developing drugs for central nervous system (CNS) disorders remains the most challenging area in drug discovery, accompanied with the long timelines and high attrition rates. With the rapid growth of biomedical data enabled by advanced experimental technologies, artificial intelligence (AI) and machine learning (ML) have emerged as an indispensable tool to draw meaningful insights and improve decision making in drug discovery. Thanks to the advancements in AI and ML algorithms, now the AI/ML■driven solutions have an unprecedented potential to accelerate the process of CNS drug discovery with better success rate. In this review, we comprehensively summarize AI/ML■powered pharmaceutical discovery efforts and their implementations in the CNS area. After introducing the AI/ML models as well as the conceptualization and data preparation, we outline the applications of AI/ML technologies to several key procedures in drug discovery, including target identification, compound screening, hit/lead generation and optimization, drug response and synergy prediction, de novo drug design, and drug repurposing. We review the current state■of■the■art of AI/ML■guided CNS drug discovery, focusing on blood–brain barrier permeability prediction and implementation into therapeutic discovery for neurological diseases. Finally, we discuss the major challenges and limitations of current approaches and possible future directions that may provide resolutions to these difficulties.